Simulation of Electronic Properties of a Quantum Dot in Transistor Geometry at Varying Temperatures

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By

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DECLARATION

I do hereby declare that the thesis titled "Simulation of Electronic Properties of a Quantum Dot in Transistor Geometry at varying Temperatures " is submitted to the Department of Mathematics and Natural Sciences of BRAC University in partial fulfilment of the requirements for the degree Bachelor of Science in Physics. This research is the work of my own and has not been submitted elsewhere for award of any other degree or diploma. Every work that has been used as reference for this work has been cited properly.

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Abstract

Electrical conduction is the flow of electron due to a force applied by an electric field. In bulk material, conduction process obeys Ohm's law. The law states that current is proportional to applied voltage. But nano-sized objects behave differently. At these range quantum effects modify the electronic conduction properties and exhibit a staircase-like conduction. This is also known as Coulomb staircase. In our work, electronic properties of a quantum dot was investigated in transistor geometry. As a device a simplified Single Electron Transistors (SET's) model has been considered, which is made of a quantum dot connected through two tunneling junctions to a source and a drain electrode, and capacitively coupled to a gate electrode. Single-Electron Transistors are often discussed as elements of nanometer scale electronic circuits because they can be made very small and they can detect the motion of individual electrons. A Python program has been developed based on rate equations and $IvsV$ characteristic graph as a function of temperature has been obtained using numerical calculation. Then radius of the quantum dot has been determined at a temperature when the QD is shifted away form quantum regime and falls into classical regime.

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Though only my name appears on the cover of this dissertation, there are many people who contributed to its production. I owe my gratitude to all those people who have made this dissertation possible and because of whom my under-graduation experience has been one that I will never forget.

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Contents

Chapter 1

Electrical Conductivity of Metals

The electrical conductivity is the ability of a substance to conduct an electric current and has the properties of inverse of resistivity. When an electrical potential V is applied across a piece of material, a current of magnitude I flows. In most metal, at very low values of V,under same physical conditions the current is proportional to V and can be described by Ohm's Law.

$$I = \frac{V}{R}$$

Where R is the electrical resistance. R depends on the geometry of the materials and on the intrinsic resistivity of the material.

Current is a continuous flow of a charged particle that implies either ion or electrons which get involved in this motion. In most materials, current is carried by the electron. In ionic crystals, charge carriers are ions. Only in liquids, both of these types of particle take part in electrical conduction.

In 1900, P.Drude first proposed a model that explains how electronic transportation happens inside a metal. That model was constructed based on the kinetic theory of gases. He used the concepts of ideal gases to visualize the properties of electron movements inside a solid bulk material. Electrons are constantly moving within the boundary of bulk material's vol-

ume and bouncing on and off inside the metal wall in a way very similar to "the ball bouncing in pinball machine arcade game ".

1.1 Drude's Model

The assumptions Drude's model is based on are stated below :

1. We are considering electron ion interaction as instantaneous, uncorrelated events.
2. An electron will travel in a straight line from one point to another point with respect to time.
3. We assume the interval in between two consecutive collision is τ. Probability of collision in a given time dt is denoted by $\frac{dt}{\tau}$. τ does not depends on electrons position and momentum.
4. The temperature will remain conserved throughout the process.

When electrons move inside a bulk material and since we are eliminating all other interaction except collision, we will trivially observe change in momentum after a collision. Let us assume at a time t the momentum of electron is $\vec{\rho}(t)$ and at a time $t + dt$ momentum becomes $\vec{\rho}(t + dt)$.

By third assumption, we could write the probability of collision as $P_c = \frac{dt}{\tau}$, assuming that we are calling probability of collision as P_c.

$\vec{\rho_c}(t + dt) = 0$, if there is no collision occurred at a time $(t + dt)$.

Since the probability should add up to 1 we could write $P_c + P_{nc} = 1$ where P_{nc} is probability of no collision.

So we can write :

$$P_{nc} = (1 - P_c)$$
$$P_{nc} = (1 - \frac{dt}{\tau}) \qquad \because P_c = \frac{dt}{\tau}$$

In case of no collision, after at time $(t + dt)$, the momentum of an electron would be :

$$\begin{aligned}\vec{\rho}(t + dt) &= \vec{\rho}(P_c + P_{nc})(t + dt) \\ &= P_c\vec{\rho_c}(t + dt) + P_{nc}\vec{\rho}_{nc}(t + dt) \\ &= (1 - \frac{dt}{\tau})(\vec{\rho}(t) + Fdt)\end{aligned}$$

By taking the time derivative of $\rho(t + dt)$ at $(t + dt)$ we can write :

$$\begin{aligned}\frac{\vec{\rho}(t)}{dt} &= \frac{\vec{\rho}(t + dt) - \vec{\rho}(t)}{dt} \\ &= \frac{\vec{\rho}(t) - \vec{\rho}(t)\frac{dt}{\tau} + \vec{F}dt - \vec{F}\frac{dt^2}{\tau}}{dt}\end{aligned}$$

Neglecting second order derivative dt^2 terms we can write :

$$\frac{\vec{\rho}(t)}{dt} = -\frac{\vec{\rho}(t)}{\tau} + \vec{F}(t)$$

Drude's model qualitively explains the phenomenon of electrical resistance and gives reliable values for the conductivity.

Despite the successes of Drude's theory, there are some features of electrical conductivity that could not be understood using Drude's Model. For instance, Drude's model fails to explain why different metal has different conductivities and why electron's movements varies from one metal to another or in alloys?

1.2 Bloch's Theorem

After 25 years of Drude's model, F.Bloch solved the quantum mechanical equation for an electron in a perfect crystal lattice. We have been treating electron as totally free. Now we introduce a periodic potential $V_{(r)}$. A periodicity appears because ions are arranged inside a material with a periodicity of their Bravais lattice. The underlying translational periodicity(T)of the lattice is defined by the primitive lattice translational vector.

$$\vec{T} = n_1\vec{a_1} + n_2\vec{a_2} + n_3\vec{a_3}$$

Where n_1, n_2, n_3 are integers and $\vec{a_1}, \vec{a_2}, \vec{a_3}$ are three non coplanar vectors.

Now $V(r)$ must be periodic.

$$\vec{V}(r+T) = \vec{V}(r)$$

The periodic nature of $\vec{V}(r)$ also implies that the potential might be expressed as Fourier's series.[9]

$$\vec{V}(r) = \sum_G V_G e^{i\vec{G}.\vec{r}}$$

Where G is a set of vectors and V_G is Fourier's coefficient.

From above equation and taking the periodicity in consideration we can set the condition as

$$e^{i\vec{G}.\vec{T}} = 1, \vec{G}.\vec{T} = 2p\pi$$

Where p is an integer. As $T = n_1\vec{a_1} + n_2\vec{a_2} + n_3\vec{a_3}$ implies that

$$\vec{G} = m_1\vec{A_1} + m_2\vec{A_2} + m_3\vec{A_3}$$

Where the m_j are integers, and the A_j are three non coplanar vectors defined by

$$\vec{a_j}\vec{A_l} = 2\pi\delta_{jl}$$

Using very simple reasoning we have shown that the existence of a lattice in r-space automatically implies the existence of lattice in k space.

The vectors $\vec{G}$ define the reciprocal lattice and the $\vec{A_j}$ represents the primitive translational vector. However periodicity in the k-space symmetry also implies that the all information will be contained in the primitive unit cell of reciprocal lattice, known as the first Brillouin zone. The first Brillouin has the k-space volume.

$$\vec{V_{k3}} = \vec{A_1} \cdot \vec{A_2} \times \vec{A_3}$$

Now we need to derive a suitable set of functions with which we can describe the motion of electrons through a periodic potential. These functions should reflect the translational symmetry properties of the lattice; and to do this we use Bornvon Karman periodic boundary conditions. We choose a plane wave

$$\phi(\vec{r}) = e^{(\vec{k}\cdot\vec{r}-\omega t)}$$

Which is subject to boundary conditions and also include the symmetry of the crystal

$$\phi(\vec{r} + N_j\vec{A_j}) = \phi(\vec{r})$$

Where j = 1, 2, 3 and $N = N_1, N_2, N_3$ are the number of primitive unit cells in the crystal. N_j is the number of unit cells in the jth direction.

The boundary condition also implies that

$$e^{iN_j\vec{k}\cdot\vec{A_j}} = 1$$

For j = 1, 2, 3. Comparing this with previous Equation suggests that the allowed wave vectors are

$$\vec{k} = \sum_{j=1}^{3} \frac{m_j}{N_j}\vec{A_j}$$

Each time m_j changes by one, we generate a new state.

Therefore, the volume of k-space occupied by one state

$$\frac{\vec{A_1}}{N_1}.\frac{\vec{A_2}}{N_2}\times\frac{\vec{A_3}}{N_3}=\frac{1}{N}\vec{A_1}\cdot\vec{A_2}\times\vec{A_3}$$

Comparing this with last equation shows that the Brillouin zone always contains the same number of k-states as the number of primitive unit cells in the crystal.

This fact has immense importance, it is the key factor in determining whether a material is an insulator, semiconductor or metal.

The Schrodinger equation for a particle of mass m in the periodic potential $V(r)$ may be written as :

$$H\psi=\{-\frac{\hbar^2\nabla^2}{2m}+V(r)\}\psi=E\psi$$

As before, we write the potential as a Fourier series

$$\vec{V}(r)=\sum_G\vec{V_G}e^{i\vec{G}\cdot\vec{r}}$$

Where G is the reciprocal lattice vectors. We are at liberty to set the origin of potential energy Wherever we like; as a convenience for later derivations we set the uniform background potential to be zero, i.e

$$V_0\equiv 0$$

We can write the wave function ψ as a sum of plane waves obeying the Bornvon Karman boundary conditions

$$\psi(r)=\sum_{\vec{k}}C_{\vec{k}}e^{i\vec{k}.\vec{r}}$$

This ensures that ψ also obeys the Born-von Karman boundary conditions. We can now substitute the wave function and the potential into

the Schrodinger equation to give

$$\sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} C_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} + \{\sum_{\vec{G}} V_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}\}\{\sum_{\vec{k}} C_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}\} = E \sum_{\vec{k}} C_{\vec{k}} e^{i\vec{k}.\vec{r}}$$

The potential energy term can be rewritten as

$$\vec{V}(r)\psi = \sum_{\vec{G},\vec{k}} V_{\vec{G}} C_k e^{i\vec{G}+\vec{k}\vec{r}}$$

Where the sum on the right-hand side is over all $\vec{G}$ and $\vec{k}$. As the sum is over all possible values of $\vec{G}$ and $\vec{k}$, it can be rewritten as

$$\vec{V}(r)\psi = \sum_{\vec{G},\vec{k}} V_{\vec{G}} C_{\vec{k}-\vec{G}} e^{i\vec{k}.\vec{r}}$$

Therefore, the Schrodinger equation becomes

$$\sum_{\vec{k}} e^{i\vec{k}.\vec{r}} \{(\frac{\hbar^2 \nabla^2}{2m} - E) C_{\vec{k}} + \sum_{\vec{G}} V_{\vec{G}} C_{\vec{k}-\vec{G}}\} = 0$$

It is going to be convenient to solve Schrodinger equation for first Brillouin zone and apply Bornvon Karman boundary conditions to see that only C_k coefficient is needed to explain the wave function. Here k is the allowed wave vectors by Bornvon Karman boundary conditions.

Now we define $\vec{k}$ such way that $\vec{k} = \vec{q} - \vec{G}$ where $\vec{q}$ lies inside the first Brillouin zone and $\vec{G}$ is general reciprocal vectors. Substituting this new value withψ_k we could find wave function for each distinct value of $\vec{q}$.

$$\begin{aligned}
\psi_q(\vec{r}) &= \sum_{\vec{G}} C_{\vec{q}-\vec{G}} e^{i(\vec{q}-\vec{G}).\vec{r}} \\
&= e^{i\vec{q}.\vec{r}} \sum_{\vec{G}} C_{\vec{q}-\vec{G}} e^{i\vec{G}.\vec{r}} \\
&= e^{i\vec{q}.\vec{r}} u_{j,\vec{q}}
\end{aligned}$$

This $u_{j,q}$ term represents the periodicity of lattice which produces a set of electron states with a particular character. This is the basis of our idea of an electronic band.

The number of possible wave functions in this band is given by the number of distinct q, i.e. the number of Born-von Karman wave vectors in the first Brillouin zone.

Therefore, the number of electron states in each band are just $2\times$(the number of primitive cells in the crystal), where the factor two has come from spin-degeneracy.

This leads us to Blochs theorem. "The eigenstates ψ of a one-electron Hamiltonian $H = \frac{\hbar^2\nabla^2}{2m} + V(r)$ where $V(r+T) = V(r)$ for all Bravais lattice translation vectors T can be chosen to be a plane wave times a function with the periodicity of the Bravais lattice. "

The ground state of a system of Bloch electrons can be constructed by filling up energy levels just as in the free electron case. To count each level only once, k needs to be limited to a single primitive cell of the reciprocal lattice, typically the first Brillouin zone. The allowed k values are still spaced discretely, even though $\epsilon_n(k)$ are continuous functions of k. Since the volume of the Brillouin zone is $\frac{8\pi^3}{\upsilon_c}$ and $\nabla k = \frac{8\pi^3}{V}$, the number of levels per band is $\frac{V}{\upsilon_c}$. Which gives $2N$ electron states per band.

Depending on the number of valence electrons Z per cell υ_c and the band structure $\epsilon_c(k)$, one may obtain completely filled or partially filled bands. The Fermi surface is obtained from the condition that

$$\epsilon_n(k) = \epsilon_F$$

If some bands are completely filled and all others remain empty, the gap between the highest occupied level and the lowest unoccupied level is called the band gap. In this case, there is no Fermi surface. This may happen - but does not need to happen - if Z is even. If Z is odd, there are always partially filled bands and a Fermi surface is formed. If the material has a Fermi surface, it also has metallic properties.

Now, in order to obtain both qualitative and quantitative result then we need to consider the different energy levels of an electron. To begin

with, let us remind ourselves of the restriction which governs the energy levels of an isolated atom. This can be summarized by the following statements:

1. Four parameters are used to explain the properties of electrons in an atom, which are denoted by n, l, m_l, and m_s. Where n is principle quantum number, l takes the integer values from 1 to $(n-1)$, m_l is allowed integer values from $-l$ and $+l$ and m_s can be -1/2 to +1/2.

2. The electrons are only allowed to occupy certain discrete energy levels, which we label using the quantum numbers n and l .

3. The occupancy of these levels are determined by the Pauli's exclusion principle which states that each electron must possess a unique set of quantum numbers.

If we apply this rule to any atom, we will find that electrons are arranged according to their shell numbers. However in a solid, atoms are not isolated. In fact they are closely attached to a large number of atoms. Therefore the electrons are not remained as a property of an atom, instead they share their outer shell electrons to create a covalent bond with other atoms and creates energy band. The energy band structure plays much the same role as the atomic energy orbital level does for an atom.

As we know from "aufbau principle " the electrons tends to remain in lowest energy level. The highest energy level, partially filled lowest energy level and the gap between them determines the tendency of electrons movement in solid bulk materials as well as clarifies the concept about why different metal and alloys inherits different conductivity. In case of partially filled energy band, we know electrons tend to occupy lowest available energy level. So if there are N electrons in a band we can assume $\frac{N}{2}$ lowest energy levels are occupied. In this case, consideration of a statistical distribution is necessary and the distribution was first determined by Enrico Fermi and Paul Dirac in 1926.

1.3 Fermi-Dirac Distribution Function

To derive the Fermi-Dirac distribution function, we start from a series of possible energies, labeled E_i. At each energy, we can have g_i possible states and the number of states that are occupied equals $g_i f_i$, where f_i is the probability of occupying a state at energy E_i. We also assume that the number of possible states is very large, so that the discrete nature of the states can be ignored. The number of possible ways- called configurations- to fit $g_i f_i$ electrons in g_i states, given the restriction that only one electron can occupy each state, equals:

$$W_i = \frac{g_i!}{(g_i - g_i f_i)! g_i f_i!}$$

This equation is obtained by numbering the individual states and exchanging the states rather than the electrons. This yields a total number of $g_i!$ possible configurations. However since the empty states are all identical, we need to divide by the number of permutations between the empty states, as all permutations cannot be distinguished from each other and can therefore only be counted once. In addition, all the filled states are indistinguishable from each other, so we need to divide also by all permutations between the filled states, namely $g_i f_i$.

The number of possible ways to fit the electrons in the number of available states is called the multiplicity function. The multiplicity function for the whole system is the product of the multiplicity functions for each energy E_i:

$$W = \prod_i W_i = \prod_i \frac{g_i!}{(g_i - g_i f_i)! g_i f_i!}$$

Using Stirling's approximation, one can eliminate the factorial signs, yielding:

$$\ln W = \sum_i \ln W_i = \sum_i [g_i \ln g_i - g_i(1 - f_i) \ln(g_i - g_i f_i) - g_i f_i \ln g_i f_i]$$

The total number of electrons in the system equals N and the total energy of those N electrons equals U. These system parameters are related

to the number of states at each energy g_i, and the probability of occupancy of each state f_i, by :

$$N = \sum_i g_i f_i$$
$$U = \sum_i E_i g_i f_i$$

According to the basic assumption of statistical thermodynamics, all possible configurations are equally probable. The multiplicity function provides the number of configurations for a specific set of occupancy probabilities f_i. The multiplicity function sharply peaks at the thermal equilibrium distribution since this is the most likely distribution of the system and must therefore be associated with the largest number of "equally probable " configurations. The occupancy probability in thermal equilibrium is therefore obtained by finding the maximum of the multiplicity function W, while keeping the total energy and the number of electrons constant.

For convenience, we maximize the logarithm of the multiplicity function instead of the multiplicity function itself. According to the Lagrange method of undetermined multipliers, we must maximize the following function :

$$\ln W - a \sum_j g_j f_j - b \sum_j E_i g_i f_i$$

Where a and b need to be determined. The maximum of the multiplicity function W is obtained by :

$$\frac{\partial}{\partial g_i f_i} \Big[\ln W - a \sum_j g_j f_j - b \sum_j E_i g_i f_i \Big] = 0$$

Which can be solved, yielding :

$$\ln \frac{g_i - g_i f_i}{g_i f_i} - a - b E_i = 0$$

Or

$$f_i = f_{FD}(E_i) = \frac{1}{1 + \exp(a + b E_i)}$$

Which can be written in the following form

$$f_{FD}(E_i) = \frac{1}{1 + \frac{E_i - E_f}{\beta}}$$

With $\beta = \frac{1}{b}$ and $E_f = \frac{-a}{b}$. The symbol E_f was chosen since this constant has units of energy and will be the constant associated with this probability distribution. Taking the derivative of the total energy, one obtains:

$$dU = \sum_i E_i d(g_i f_i) + \sum_i g_i f_i dE_i$$

Using Lagrange equation this can be rewritten as

$$dU = \beta dB(\ln W) + \sum_i g_i f_i dE_i + E_i$$

Any variation in the E_i can only be caused by a change in volume, so that the middle term can be linked to a volume variation dV.

$$dU = \beta dB(\ln W) + \Big[\sum_i g_i f_i dE_i + E_f dN\Big] dv + E_f dN$$

Comparing this to the thermodynamic identity:

$$dU = TdS - PdV + \nu dN$$

One finds that $b = kT$ and $S = k \ln W$, where k is a constant that must be determined. The energy, E_f, equals the energy associated with the particles, namely the electro-chemical potential, m. The comparison also identifies the entropy S, as being proportional to the logarithm of the multiplicity function, W. The proportionality constant, k is known as Boltzmann's constant. The Fermi-Dirac distribution function then becomes:

$$f_{FD} = \frac{1}{1 + \frac{E - E_f}{kT}}$$

The Fermi-Dirac distribution is also known as the "Fermi factor ". Note that in proper quantum terms, it gives the probability that a state is occupied by an electron.

Chapter 2

Nanoparticles and Quantum Dots

2.1 Nanoparticles

Nanoparticles are the rudimentary component in the invention of nanostructure. The size of objects that we usually interact in real life is far larger than nano scale object. Their physical properties remain persistent regardless of their size and all could be explained using Newton's laws of motion. As we approach to smaller scale regions, to understand how things act beyond our naked eye with the help of microscopic view, we perceive that physical properties depend on sizes and shapes.

Quantum confinement in semiconductor particles, surface plasmon resonance in some metal particles and super magnetism in magnetic materials become apparent because of size dependencies.[5]

Nanotechnology might be a finding of modern science, but nanoparticles have quite long history. The optical properties of nanoparticle fascinates artisans and have been used from time immemorial for building radiant sculpture and shiny pottery. Lycurgus cup was one of the oldest specimen made by using dichoric glass which contains metal crystals of Ag and Au (size of $70nm$). These crystal gives unique color properties. The history of the

nanoparticle from ancient times to the Middle Ages has been summarized by Daniel and Astruc. At that time physician used soluble gold as a portion to cure various human disease. Nanotechnology is easily conspicuous in various old churches painting. From after middle ages to early twentieth century scientist did experiment and researched with ultra fine gold particles, but due to lack of advanced technology proper understanding about ultra fine particle was not easier. At 1937 Scanning electron microscope (SEM) was invented by M. Von Ardenne. Twenty two years later Richard P. Feynman, a physicist at CalTech, forecasted the advent of nanomaterials. In one of his lectures he said, qThere is plenty of room at the bottom and suggested that scaling down to nano level and starting from the bottom was the key to future technology and advancement.[6]

As the field of nanotechnology advanced, noble nanomaterials become apparent having different properties as compared to their larger counterparts. Many physical properties of materials, especially the melting point, change when the physical size of the material approaches the micro and nano scales.[12]

Interesting magnetic properties have also been observed in small clusters. In a cluster the magnetic moment of each atom will interact with the moments of the other atoms, and can force all the moments to align in one direction with respect to some symmetry axis of the cluster the cluster will have a net magnetic moment, it will be magnetized. As cluster size decreases it therefore becomes easier for them to exhibit ferromagnetic behaviour. In some cases, even clusters made up of nonmagnetic atoms can have a net magnetic moment. For instance rhenium clusters show a pronounced increase in their magnetic moment when they contain less than 20 atoms. For clusters with less than 15 atoms these moments are fairly large.

One of the most fascinating and useful aspects of nanomaterials is their optical properties. Applications based on optical properties of nanomaterials include optical detector, laser, sensor, imaging, phosphor, display, solar cell, photocatalysis, photoelectrochemistry and biomedicine. The optical properties of nanomaterials depend on parameters such as feature size, shape, surface characteristics, and other variables including doping and interaction with the surrounding environment or other nanostructures. Likewise, shape can have dramatic influence on optical properties of metal nanostruc-

tures.

In general nanoparticles are particles with at least one dimension from $1nm$ to $100nm$ in size. [10] These can include, e.g. fullerens, metal clusters (agglomerates of metal atoms), large molecules, such as proteins, and even hydrogen-bonded assemblies of water molecules, which exist in water at ambient temperatures. Nanoparticles represent a state of matter in the transition region between bulk solid and single molecule.

Nanomaterials can be nano scale in one dimension (e.g. surface films), two dimensions (e.g. strands or fibers), or three dimensions (e.g. particles).[2] They can exist in single, fused, aggregated or agglomerated forms with spherical, tubular, and irregular shapes.[1] Common types of nanomaterials include nanotubes, dendrimers, quantum dots and fullerenes. According to Richard W.Siegel, Nanostructured materials are classified as Zero dimensional, one dimensional, two dimensional, three dimensional nanostructures.

Zero dimensional nanomaterials have nano-dimension in all three directions. Metalic nanoparticles including gold and silver nanoparticles and semi conductor such as quantum dots are the perfect example of this kind of nanoparticles. Most of these nanoparticles are spherical in size and diameter of these particles will be in the $1 - 50nm$ range.

In one dimensional nanostructure, one dimension of the nano structure will be outside of nano meter range. These include nanowires, nanorods and nanotubes. These nanomaterials are long but with diameter of only a few nanometer. Nanowire and nanotubes of metals, oxides are few example of this kind of materials.

In two dimensional nanostructure, two dimensions are outside the nanometer range. These include different kind of nano films such as coatings and thin film multilayer, nano sheets or nano walls. The area of the nano films can be large, but thickness is always in nano scale range.

All dimensions of three dimensional nanostructure are outside of nanometer range. These includes bulk materials composed of individual blocks which are in the nanometer scale.

Fig-2.1[15] illustrates the conductance of different sizes nanoparticles. As we see quantum dot belongs to zero dimensional nanoparticle and it has discrete conductance peak which results in discrete current flow.

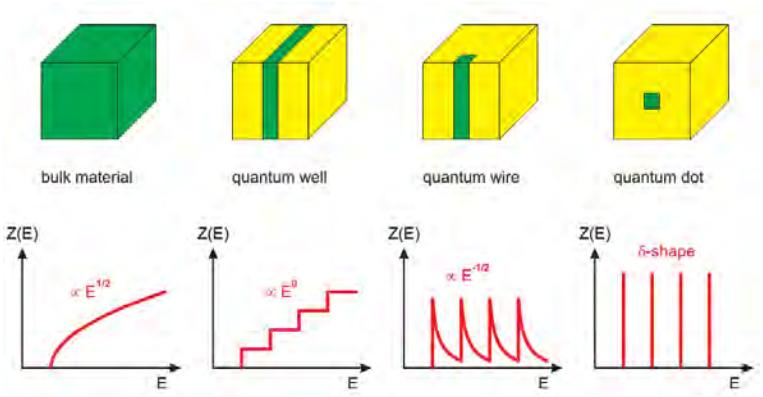

Figure 2.1: Spatial confinement of semiconductor structures and corresponding electronic states

2.2 Quantum Dots

"Quantum dots are man-made "droplets "of charge that can contain anything from a single electron to a collection of several thousand. By confining electrons in three dimensions inside semiconductors, quantum dots can recreate many of the phenomena observed in atoms and nuclei, making it possible to explore new physics in regimes that cannot otherwise be accessed in the laboratory. "[11]

As we have already discussed, nanoparticles have larger surface-to-volume ratio and the number of surface atoms may be similar to or higher than those located in the crystalline lattice core, therefore the surface properties are no longer negligible. When no other molecules are adsorbed onto the nanocrystallites, the surface atoms are highly unsaturated and their electronic contribution to the behaviour of the particles is totally different from that of the inner atoms. These effects may be even more marked when the surface atoms are tightly bound. This leads to different electronic transport

and catalytic properties of the nanocrystalline particles.

Another phenomenon, which occurs in metal and semiconductor nanoparticles, is totally an electronic effect. The band structure gradually evolves with increasing particle size, i.e. molecular orbital convert into delocalized band states. In a metal, the quasi-continuous density of states in the valence and the conduction bands splits into discrete electronic levels, the spacing between these levels and the band gap increasing with decreasing particle size.

In the case of semiconductors, the phenomenon is slightly different, since a band gap already exists in the bulk state. However, this band gap also increases when the particle size is decreased and the energy bands gradually convert into discrete molecular electronic levels.[16] If the particle size is less than the De Broglie wavelength of the electrons, the charge carriers may be treated quantum mechanically as qparticles in a box, where the size of the box is given by the dimensions of the crystallites.[13] In semiconductors, the quantization effect that enhances the optical gap is routinely observed for clusters ranging from $1nm$ to almost $10nm$. Metal particles consisting of 50 to 100 atoms with a diameter between $1nm$ and $2nm$ start to lose their metallic behaviour and tend to become semiconductors.

Particles that show this size quantization effect are sometimes called Q-particles or quantum dots. QD's are often also called mesoscopic atoms or artificial atoms to indicate that the scale of electron states in QD's is larger than the lattice constant of a crystal. However, there is no rigorous lower limit to the size of a QD, and therefore even macromolecules and single impurity atoms in a crystal can be called QDs.[7]

The analysis and understanding of the electronic properties that lead to these applications involve quantum confinement effects of the carriers, which crucially requires the accurate determination and characterization of the electron and hole energy levels.

The conduction band and valance band in a quantum dot are described by an effective Schrdinger equation :

$$\frac{-\hbar^2\Delta^2}{2m_0m^*}\psi(r) + V(r)\psi = E\psi(r)$$

Where the effective mass m^* and the confining potential $V(r)$ depend on the material and the band of interest. m_0 is the free electron mass and $\bar{h}$ is the reduced Planck constant. ψ is called the envelope function and E is the energy of the state measured relative to relevant band edge. In the simplest model, the potential V is given by the band edge discontinuity between the QD and the surrounding material.

QD's are small compare to the bulk excitation of Bohr radius, the Coulomb interaction may be treated perturbatively. The commonly used first-order perturbation theory gives an electron-hole binding energy of $1.786e^2\epsilon R$ where e is the elementary charge and ϵ is the dielectric constant responsible for screening of the Coulomb interaction. The above considerations lead to a simple expression for the ground state energy of a confined electron-hole pair in spherical QD's:

$$E_{exc} = E_g + \frac{\hbar^2\pi^2}{2m_0R^2}(\frac{1}{m_e} + \frac{1}{m_h}) - \frac{1.786e^2}{\epsilon R}$$

This simple theory very well captures the qualitative effects of confinement, viz., discrete nature of excitation energies, a blue shift of the absorption edge that increases as the size of the QD is reduced, and the enhancement of the Coulomb interaction with decreasing QD size. This model has also been generalized to two-electron states including the electrostatic potential of image charges. However, its quantitative validity is extremely limited because of two major shortcomings. First, the effective mass picture is valid only close to the band edges where the bands are parabolic. However, particularly in small QD's, where the confinement energy is larger, the energy levels are pushed deep into the bulk bands where non parabolicity effects are important. Second, in most semiconductors of interest, the valence band edge is degenerate leading to mixing of bands by the confinement potential. Proper treatment of band-mixing is important even for a qualitatively correct description of the electronic wave functions, as well as for several important properties such as oscillator strengths for optical absorption.

Chapter 3

Transistors

We have already discussed briefly about conduction in metals. Based on how good a material can conduct current, we can divide them into three groups i.e. conductor, semiconductor, insulator. Semiconductors are kind of materials that inherits some characteristics of metal and some characteristic of insulator.

Conductor type metal has one or two electron per atom. Generally these electrons moves towards opposite direction if we apply electric field. Insulators also have many electrons in them, but the electrons cannot move. Some of them are trapped in individual atoms and can't get away from them. Others are nominally free to move about, but are locked in place by qgridlock.

"Energy gap ", which means the gap between valance band and conduction band, is zero in good conductor and gap is large in insulator. It is impossible for an electron to jump from valance band to conduction band in insulator.

The resistivity and resistance of most conductor increases with temperature, but semiconductor like silicon resistance goes down. When an electron make this jump to conduction band, the parent atom becomes deficient, and most text book refers them as hole because it can be filled by another electron. When current flows in a semiconductor, an electron can migrate from atom to atom. So these holes appears to migrate opposite direction to

the electron and these constitutes a current as well.

Natural semiconductor are called intrinsic semiconductor. When they are modified by manufacturing process to give them enhanced properties, they are then called extrinsic. Extrinsic semiconductor are produced by doping them to enhance their conductivity. The conductivity of semiconductor, like silicon can be increased by adding small amount of impurities that have roughly same atomic size, but more or fewer electron than semiconductor. This process is known as doping. If adding impurity in semiconductor makes the material positively charged then materials become p-type semiconductor and while negatively charged makes n-type semiconductor.

So p-type semiconductor has hole surpluses and n-type semiconductor has electron surpluses. As a result if n-type and p-type were brought together to create junction then the current can only flow one direction from n-type to p-type. Flow cannot go reverse direction. This type of combined semiconductor is called diode.

Now if we add another semiconductor material to a diode to create one more junction, then as a whole the combination is called transistor. Transistor either can be n-p-n or p-n-p. The formation of this kind of sequence based on their function is dubbed as emitter-source-collector or in our case source-gate-drain. In operation drain is reverse biased relative to base so that no current flows even if the voltage is large. On the other hand if the source is forward biased, then current can flow even in relatively small voltage.

Before the invention of transistor, electron tubes were a basic component for electronics throughout the first half of the twentieth century. Electron tube was larger than transistor and required to heat up to work properly. It was used largely by the radio, television, radar, telephone company. It was only after 1956 appeared that transistor would immediately revolutionized the electronics industry, because large demand for new electronic devices and whole productions was difficult to overcome using old devices. After that electrical industry has seriously turned to this modern age technology.

Another interesting thing about transistor is that we can make the size of gate very thin. It could be scaled down to nanometre range. By

scaling down, we could make island small enough to create quantum dot so that single electron can only stay in this island. A quantum dot with single electron shows negative charge. As a result if another electron tries to come to that place, it will feel repulsion force due to electric field created by single electron. The repulsion force is effectively measured by the equation:

$$E = \frac{e^2}{2C}$$

From above equation it is clearly visible if capacitance becomes very small the charging energy will be high. So electron movement from source will be restricted by the charging energy which works like a barrier for an electron. Thus current flow might become quantized and electrons cannot jump into quantum dot unless it releases electron to drain. It's worth mentioning here that two conditions must not be ignored for this process that coulomb energy must be greater than thermal fluctuations and electron should be localized only on the island.

3.1 Single Electron Transfer

Charge flow in metal and semiconductor is a continuous process because conduction electron are not localized in a specified location. Electrons are spread over the whole surface area which forms quantum fluid that can be shifted by arbitrary small amount. The small variations of the charge Q on a capacitor with potential difference $U = \frac{Q}{C}$ illustrates this property. The charge can be any fraction of ϵ of the charge quanta e.

There exists however a solid state device which can transfer electrons in discrete manner. It consist of two metallic electrodes, as named as source and drain, separated by an insulating layer so thin that can traverse electron by quantum tunneling.[14] Tunneling can be all or nothing process because electron could not spend much time in insulating layer. If one applies a voltage V to such a tunnel junction then electron will tunnel across the insulator at a rate give by $\frac{V}{eR_t}$. Here R_t is the tunnel resistance depends on the thickness and area of the insulating barrier. It is important to stress that the transport of an electron in tunnel junction and in a metallic resistor

are fundamentally different, even though the current-voltage characteristic is linear in both cases. Charge flows continuously align the resistor whereas it flows across the junction in packets of e. It is obvious a tunnel junction provides the means to extract electrons one at a time from an electrode.

However, the stochastic nature of tunneling makes it difficult to control electron transport from upstream electrode to downstream electrode. To gain more control over this nature, we usually add another gate electrodes in between source and drain electrodes. We can call such isolated electrode, in which electrons can enter and leave only by tunneling, an island. The island is coupled electrostatically to the rest of the device.

Suppose furthermore, that the island dimensions are small enough that the electrostatic energy $E_c = \frac{e^2}{2C_\Sigma}$ of one excess electron on the island is much larger than the characteristic energy k_bT of thermal fluctuation. At temperatures below $1K$, no current can pass through the island with low bias voltage. This effect is known as the Coulomb blockade, which is the result of the repulsive electronelectron interactions on the island. Coulomb blockade is the repelling energy of previous electron present in the island to the next electron coming towards the island. The concept of Coulomb blockade refers to the phenomenon that tunneling through an island may be inhibited at low temperatures and small applied voltage. The reason is that the addition of a single electron to such a system requires an electrostatic charging energy.

In metals, the Coulomb-blockade oscillations are essentially a classical phenomenon, since the energy spectrum of the confined region may be treated as a continuum. However, this is not the case in semiconductor nanostructures which have dimensions comparable to the Fermi wave length.

3.2 Single Electron Transistor

Single electron devices (SEDs) are based on the controllable single electron transfer between small conducting islands. The single-electron transistor describes a single electron transport through a quantum dot. A quantum dot is a semiconducting nanoparticle whose electrons are confined in all three spatial dimensions. There are many variations to the structure of the single-

electron transistor. The main components of the single- electron structure are shown in fig-3.1.[3]

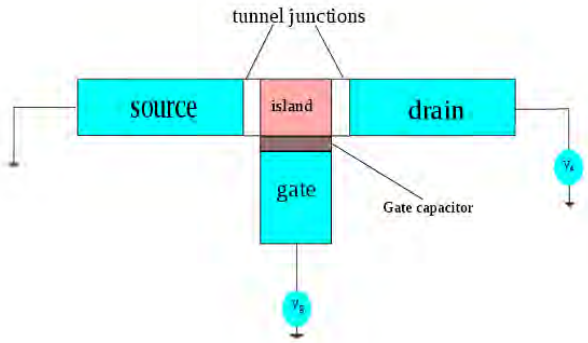

Figure 3.1: Single Electron Transistor

The island is the quantum dot which is connected to the drain and source terminals. Electron exchange occurs only with the drain and source terminals, which are connected to current and voltage meters. The gate terminal provides electrostatic or capacitive coupling. When there is no coupling to the source and drain, there is an integer number N of electrons in the quantum dot(island). The total charge on the island is quantized and equal to qN. Since tunneling is a discrete process, the electric charge that flows through the tunnel junction flows in multiples of the charge of electrons e.

The formulation of the Coulomb blockade model is only valid, if electron states are localized on islands. In a classical picture it is clear, that an electron is either on an island or not. That is the localization is implicit assumed in a classical treatment.

However a more precise quantum mechanical analyses describes the number of electrons localized on an island N in terms of an average value, $< N >$ which is not necessarily an integer. The Coulomb blockade model requires.

$$|N - < N > |^2 \ll 1$$

Clearly, if the tunnel barriers are not present, or are insufficiently opaque, one can not speak of charging an island or localizing electrons on a quantum dot, because nothing will constrain an electron to be confined within a certain volume.[4] If tunneling is allowed between the island, drain, and source terminals, then the number of electrons N adjusts itself until the energy of the total system is minimized. The tunneling junctions (barriers) are made thick enough so that the electrons exist in the island, source, or drain, such that the quantum fluctuation in the number N due to tunneling through the barrier is much smaller than one. The electrostatically influenced electrons travelling between the source and the drain terminals need to tunnel through two junctions (barriers).

The island is charged and discharged as the electrons cross it, and the relative energies of the island containing zero or one extra electron depends on the gate voltage. Thus, the charge of the island changes by a quantized amount q. The change in the Coulomb energy associated with adding or removing an electron from the island is usually expressed in terms of the island capacitance C. The charging energy E_c can be expressed as

$$E_c = \frac{q^2}{C}$$

This charging energy becomes important when it exceeds the thermal energy k_{BT}. The time δt needed to charge or discharge the island can be expressed as

$$\Delta t = R_t C$$

Where R_t is the lower-bound tunnel resistance. From the Heisenberg uncertainty principle we have, $R_t > \frac{\hbar}{q^2}$. The quantity $\frac{\hbar}{q^2} = 25.813k$ is called the quantum resistance or quantum conductance ($G = 38.74S$).

Thus, two conditions must be met to observe the charge quantization:

$$R_t \gg \frac{\hbar}{q^2}$$

$$\frac{q^2}{c} \ll k_b T$$

The capacitance can be made small by reducing the quantum dot size since $C = 4\pi\epsilon_s R$ for a sphere and $C = 8\pi\epsilon_s R$ for a flat disc, where R is the radius and s is the permittivity of the material. The gate voltage V_g is applied to change the island electrostatic energy in a continuous manner. The total gate voltage-induced charge on the island is expressed as $q = C_g V_g$. This charge is considered continuous. By sweeping the gate voltage, the build up of induced charge will be compensated in a periodic interval due to the tunneling of discrete charges. The competition between the induced charges and the discrete compensation leads to so-called Coulomb oscillations. Consider that the gate voltage is fixed for the single-electron transistor while the drain-source voltage is varied. The current-voltage results exhibit a staircase-like behaviour known as a Coulomb stair-case.

Chapter 4

Fabrication

Experiment designers have already developed various kinds of experiment technique for wiring up a quantum dots inside transistor geometry. Scanning Probe Microscopy (SPM), two unconventional technique (e.g The Electro-deposition Technique, The nano constriction technique) and mostly popular technique the electro-migration technique.

We would like to mention briefly about all these popular and effective procedures here.

The scanning probe microscopy : This technique allows us to actually see molecule before measuring them but it requires high level instrumentation and many expertise to perform the experiments. Another drawbacks of this method which is against our purpose because of the reason that it does not have gate electrode. Therefore measuring gate voltage is not possible. In this methods a continuous metallic electrodes brought into a flexible substrate level and bend to extent until it breaks. In this way we could brought electrode length into pm level.

The electro-deposition technique : Morpurgo, A.F., C.M. Marcus, and D.B. Robinson first explains the unconventional process by positioning two electrodes together on an insulating substrate and then two electrodes are brought nearer until separation become smaller. The separation between this electrodes could be as small as $1nm$. This process combines both elec-

trochemical and lithographic process.

The naonoconstriction technique : A small hole is created with the size of a molecule in a thin small silicon nitrate membrane and two electrodes brought together around the hole to make tunnel barriers. Another process is currently done in which a molecule is pushed into a electrodes using a needle.

The electro-migration technique : The process we will follow in our work is electro-migration. This process is kind of a combination of scanning probe microscopy technique and lithography.

A continuous wire is fabricated using standard e-beam lithography. Applying large voltage $(0.5 \text{ to } 1)\upsilon$, we create a small gap typically 1 to $2nm$ in length. This small gap works as a place for gate electrode. Usually when a metallic wire kept under large density of current for over a long period of time, the ongoing process finally breaks down the wire. It creates problem for uninterrupted current. In bulk metal, atoms are closely connected to each other. Their formations are not tightly bound. Defects on their structure provides impurities, dislocations and grain boundaries.

Current flow through this structure changes electron's directions. As a result collision and scattering happens. It transfers momentum to scatterer, thus exerts a force on it. This force can cause the scatterer to move out of it's original position. Larger current density increases the number of relocation events. It will be also accelerated at higher temperature because lattice phonon will help atoms move out of their original position. This mass transport process caused by a large electric current density (electron winds) is called electro-migration.

The formation of the gap can be seen by SEM technique. In between this gap we put a molecule or quantum dots. Electronic level of these dots is controlled by gate electrodes. As a gate electrode we choose thinner, smaller and stronger electrode. We know that electrochemical potential of a quantum dot can be controlled by gate electrode. That's why we place gate electrodes as close as possible to gate electrodes(less than $50nm$). The relation between the gate capacitance and the thickness of the gate insulator will vary depending on the local device geometry and electrostatics. We are

using compound of oxide as gate electrodes.

In reality, the oxide usually fails well below $30V$ and in some cases electric current flows between the gate and the source/drain electrodes even at very low biases. This premature gate failure and gate leakage is caused by impurities and pin-holes present in the gate oxide.

To minimize this annoying possibility, one can reduce the overlap area between the gate and the source/drain electrodes.

Again, it is not a good idea to make the whole electrode structure (typical total area $0.1\ cm^2$) on top of a $30nm$ gate oxide. Instead, one can reduce the premature gate failure and gate leakage by defining two regions with different gate thickness; a small region with a thin gate oxide and all other areas with a thicker ($> 200nm$) field oxide.

Chapter 5

Simulation

5.1 Counting The Electron

Counting statistics in sequential tunneling is the mathematical process that counts the average number of electrons flows from source to drain via quantum dot island. Since it is a flow of electron, the rate equation comes to as an very handy tool in quantum electronics. Rate equation provides the statistical information about the system.

In case of quantum scenario, where energy and time has very close connection, rate equation can be expanded to gather statistical information about the distribution of energy amongst the particles. From the distribution of energy states one can demonstrate that electrons are placed over potential μ according to Boltzmann distribution.

$$n = N_e \exp^{\frac{\mu}{k_b T}}$$

No particular assumption was made in rate equation other than the fact that the particles are conserved in a phase, so that energy would be conserved automatically.

Consider then, a set of particles n_i that can exist any of N_i range which are all at energy E_i. An arbitrary range of values of integer i denotes the different energies. One can simply argue that there are N_i states available for n_i electrons. This assumption can later be contrasted with the assumption of quantum particles. The whole system supposed to be closed system with no energy lost or gained from external source. It is assumed that particles interact with only other particles at any one instant of time.

Now let us assume that there are three more energy range E_j, E_k, E_l where $(i < j < k < l)$ and situated particles are n_j, n_k, n_l respectively. Suppose then one of n_j particle exchanges its energy with similar particle of n_k at range N_k whose energy is E_k. The j particle scattered or changes state to become a l particle in one of N_l range at energy E_l. The k particle with which j particle interacted now needs to change it's state in order to conserve its energy. So the k particle moves to level i whose energy state is E_i. The initial energy equals to the final energy for this interaction requiring that

$$E_j + E_k = E_i + E_l$$

The probability of a E_j energy level particle jumping to a E_l energy level particle is proportional to the number of particle available to move and to the number of states at energy level E_l available to receive the particle. So that

$$\frac{dn}{dt}_{j\to l} \propto n_j N_l$$

The movement of E_j energy level particle to a states at energy level E_l has to be linked, through energy conservation, by allowing the particle movement from k to i. This is also proportional to the number of available particle n_k and to the number of available states E_i. So

$$\frac{dn}{dt}_{k\to i} \propto n_k N_i$$

Now combining the two rate equations and summing over all the possible states at k and i we can write

$$\frac{dn}{dt}_{j\to l} = \sum_{k,i} \{A_{jk,il}\ \ n_j n_k N_l N_i\}$$

$A_{jk,il}$ is the probability of a change per single particle at j to a single available state at l accompanied by the movement of single particle at k to a single available state i. As the same way, we can show that $A_{il,jk}$ is the probability of a change per single particle at i to a single available state at k accompanied by the movement of single particle at j to a single available state l.

$$A_{jk,il} = A_{il,jk}$$

$A_{il,jk}$ is the exactly opposite motion of $A_{jk,il}$ and it is believed that two outcome has the same probability. This justification is made by what happens by reversing time for a cloud of interacting particles where all energy accounted for in the system and no energy takes away from the system. It is supposed to be true that this "time reversal " properties carries over into all types of interaction.[8] Scattering into j is then formed similar way to scattering out. So to give the total scattering into and out as :

$$\begin{aligned}\frac{dn_j}{dt} &= \sum_{i,k,l} \{A_{jk,il}\ \ N_j N_k n_i n_l - n_j n_k N_i N_l\} \\ &= \sum_{i,k,l} \left\{ A_{jk,il}\ \ n_j n_k n_i n_l \left[\frac{N_j}{n_j}\frac{N_k}{n_k} - \frac{N_i}{n_i}\frac{N_l}{n_l} \right] \right\}\end{aligned}$$

In equilibrium $\dfrac{dn_j}{dt} = 0$ over ensemble of system. The detailed balance that is required to bring the system in equilibrium regardless mechanism of interaction is given by

$$\left(\frac{N_j}{n_j}\right)\left(\frac{N_k}{n_k}\right) = \left(\frac{N_i}{n_i}\right)\left(\frac{N_l}{n_l}\right)$$

$$\ln\left(\frac{N_j}{n_j}\right) + \ln\left(\frac{N_k}{n_k}\right) = \ln\left(\frac{N_i}{n_i}\right) + \ln\left(\frac{N_l}{n_l}\right) = f$$

By comparing above equation with the energy conversion law we can confirmed that the f must be the function of $f(E)$, with $f(E)$ and E both conserved in collision. The functional dependences of n_j over E_j gives us

$$\ln\left(\frac{N_j}{n_j}\right) = b\left(E_j - E_l\right)$$

This hold for all i, j, k, l. Here b and E_l are independent of state j. Then we can expect that the occupation of an energy state averaged over the number of ensemble given by

$$n_j = N_j \exp^{[-b(E_j - E_l)]}$$

The rate equation do not, in general give the constant value which are used, and this constant have to be determined from experiment or comparing with other theories. Comparison with ideal perfect gas gives

$$b = \frac{1}{k_b T}$$

where k_b is the Boltzmann constant and T is the temperature. The constant E_l is determined from the total number of N.

$$N = \sum_j n_j = \sum_j N_j \exp^{[-b(E_j - E_l)]}$$

$$E_l = k_b T \ln\left\{\frac{N}{\left[\sum_j N_j \exp^{\frac{E_j}{k_b T}}\right]}\right\}$$

The energy E_l provides a reference energy determined by the states and the number of particles. Above equations determine the definite value for E_l when N is known. Typically the N is fixed for metal, in that case the energy is called Fermi energy.

Now we restrict particles movement by considering Pauli's quantum restriction. In this case the available states at certain energy level is

$(N_m - n_m)$ where $m = i, j, k, l$. Therefore the new probability of the movement happening for just one particle at j and k with one vacancy at i and l is given by

$$\frac{dn}{dt}_{j\to l} = \sum_{k,i} \left\{ A_{jk,il} \;\; n_j n_k \left(N_l - n_l\right)\left(N_i - n_i\right) \right\}$$

So that the total scattering both into and out of j is given by

$$\frac{dn_j}{dt} = \sum_{i,k,l} \left\{ A_{jk,il} \left(N_j - n_j\right)\left(N_k - n_k\right) n_i n_l - n_j n_k \left(N_i - n_i\right)\left(N_l - n_l\right) \right\rangle$$

Here the system is also a closed system, with no energy being lost to or gained from any external source. All interaction in this closed system is considered to be the function of energy. So we can write

$$\ln\left(\frac{\left(N_j - n_j\right)}{n_j}\right) = b\left(E_j - E_l\right)$$
$$\ln\left(\frac{N_j}{n_j} - 1\right) = b\left(E_j - E_l\right)$$

The final result for the distribution with energy is then given as the Fermi-Dirac distribution

$$F\left(E\right) = \frac{n_j}{N_j} = \frac{1}{1 + \exp\frac{\left(E_j - El\right)}{k_b T}}$$

We are basically solving the rate equation for one level quantum dot provided by the Fermi-Dirac probability distribution function to simulate electronic transportation in nano particle at increasing temperature. The

complete set of equation for source and drain could be derived as bellow :

$$f_D = \frac{1}{1+\exp^{(\frac{\mu_{(N+1)}-\mu_D}{k_bT})}} \qquad = \frac{1}{1+\exp^{(\frac{\mu_{(N+1)}}{k_bT})}}$$

$$f_S = \frac{1}{1+\exp^{(\frac{\mu_{(N+1)}-\mu_S}{k_bT})}} \qquad = \frac{1}{1+\exp^{(\frac{\mu_{(N+1)}+|e|V}{k_bT})}}$$

$$\mu_{(N+1)} = E_0 - |e|\,\frac{C_G V_G + C_S V}{C_{total}} \qquad = -\,|e|\,\frac{C_G V_G + C_S V}{C_{total}}$$

Then the current I will be ,

$$\frac{I}{|e|} = -P_0\Gamma_s f_s + P_1\Gamma_s(1-f_s) \qquad = \frac{\Gamma_S\Gamma_D}{\Gamma_S+\Gamma_D}(f_D - f_S) \equiv \Gamma(f_D - f_S)$$

5.2 Atomistic Simulation

There are various methods to do atomistic simulation. Among all of them I wish to review some popular methods that are related to our work such as : Empirical methods, Quantum Mechanical methods, Molecular Dynamics methods, Metropolis Monte Carlo methods.

Empirical Methods is one of the most simplest and idealistic case for simulation. This methods involves simple equations that gives a reasonable description about the system. This model assumes that ion are fixed as a result they can not move. In this methods the existence of usable and appropriate function is the only part of an issue but the greater challenge is whether the parameter in the function can be tuned to appropriate values. Formally this procedure is carried out by adjusting the parameter in the model until it agrees with the experimental data. A more refined approach is to incorporate real data.

Quantum mechanical methods holds out the possibility to perform a simulation that can provide reliable results without the prior need of tuning parameters . This computational methods solve such equations for which there is no exact solution. Finding solution is a big challenge in this model. The wave function properly describe a particle in this system. So we heavily

use wave equation to simulate a particle in quantum mechanical methods. However in case of particle-particle interaction the wave function we achieve could not be assigned to individual particle. Another methods that is mostly used in today's world simulation is density functional theory. It is based on number of electron passing thorough per unit area rather than wave equation. Density functional theory describes motions of electron containing per unit area and then build the model based on that whereas wave function describes a single particle and then build the model by taking product of every participle in the system.

The molecular dynamics is simple in concept. The idea in which molecular dynamics is based on is the link between acceleration and force in Newtonian mechanics. It uses Empirical or Quantum mechanical methods to calculate the force of a particle and then convert the force into acceleration. Acceleration could be derived further using a time interval to measure velocities and positions.There are actually several algorithms in common use, giving the level of stability and accuracy required by the specific application. The result of a simulation is the evolution of the positions and velocities of an ensemble of atoms through time. It is possible to extend the set of equations to include additional dynamical variables that enable the simulations to correspond to constant temperature (variable energy) and constant pressure/stress (variable sample volume and shape).

The Monte-Carlo methods is the one that is common use in computational science, requires an algorithm for generating a new configuration by changing a previous configuration. Any change in the configuration or atomic ensemble will give a change in energy. If the energy change ΔE is negative, leading to a lowering of the energy, the change is automatically accepted. On the other hand, if the energy change is positive, the configuration is only accepted with probability $\exp^{(\frac{-\Delta E}{k_b T})}$. This procedure is repeated for a large number of steps, leading to an evolution of the ensemble through the multidimensional phase space. This approach ensures that the sampling procedure is consistent with thermodynamics; for example, states with any energy E occur with the relative probability $\exp^{(\frac{-\Delta E}{k_b T})}$. The complete set of configurations, including duplicated configurations, can be analyzed to give averaged quantities that have the correct thermodynamic weighting automatically ensured. For example, it is possible to calculate the average energy

as a function of temperature, and the variance of the energy will yield the heat capacity using the standard formulation based on fluctuations.

5.3 Why Python?

It was the first task to choose a well-structured and object-orientated programming language for our simulation. Now a days, there are lots of programming language that can do calculation what we need. i.e. C, C++, Java, FORTRAN, Python etc. Among all of them I used python for evaluating Fermi-Dirac equation because it seems to me comparatively easier to understand than other language and it demands less amount of hand written code for execution. There are some programming structural advantages unlike other language provides.

Simulation program usually needs to calculate large number of data. To handle large number of data, I store them into a Numpy array rather than normal python list.I found normal array as less precise and took large amount of time to store data and to call them whenever I need.

A NumPy array is basically described by a metadata (number of dimensions, shape, data type) and the actual data. The data is stored in a homogeneous and contiguous block of memory, at a particular address in system memory (Random Access Memory, or RAM). This block of memory is called the data buffer. This is the main difference with a pure Python structure, like a list, where the items are scattered across the system memory. This aspect is the critical feature that makes NumPy arrays so efficient.

Array computations can be written very efficiently in a low-level language like C (and a large part of NumPy is actually written in C). Knowing the address of the memory block and the data type, it is just simple arithmetic to loop over all items, for example. There would be a significant overhead to do that in Python with a list.

Spatial locality in memory access patterns results in significant performance gains, notably thanks to the CPU cache. Indeed, the cache loads bytes in chunks from RAM to the CPU registers. Adjacent items are then

loaded very efficiently (sequential locality, or locality of reference).

Data elements are stored contiguously in memory, so that NumPy can take advantage of vectorized instructions on modern CPU's, like Intel's SSE and AVX, AMD's XOP, and so on. For example, multiple consecutive floating point numbers can be loaded in 128, 256 or 512 bits registers for vectorized arithmetical computations implemented as CPU instructions.

Additionally, let's mention the fact that NumPy can be linked to highly optimized linear algebra libraries like BLAS and LAPACK, for example through the Intel Math Kernel Library (MKL). A few specific matrix computations may also be multi threaded, taking advantage of the power of modern multi core processors.

Our simulation also required some very well-known physical constant. For that reason, we took help from *Scipy* library, where all the well-known constants are available. We also use $Mathlibrary$ to get the natural epsilon value.

We created a python class which acts like a volt-meter that inputs voltage at very small interval. This class basically is our virtual volt-meter for source and drain. To apply voltage at very small rate we build a function that tells the volt-meter how small a step could be.For every voltage, we calculated chemical potential. Later we declared two separate function that can determine Fermi state for source and drain. Then we ran the whole function for several times based on the number of voltage input. The result that is produced by the Fermi-Dirac function are stored in another $Numpy$ array so that we could use them to calculate current. The difference between two Fermi state times the intrinsic broadening value produces the desired current. Python also provides a class called *Pyplot* which has a subclass called *mathplotlib.py*. We used this library to plot the numeric values.

In conclusion,I used Python because storing data in a contiguous block of memory ensures that the architecture of modern CPUs is used optimally, in terms of memory access patterns, CPU cache, and vectorized instructions.

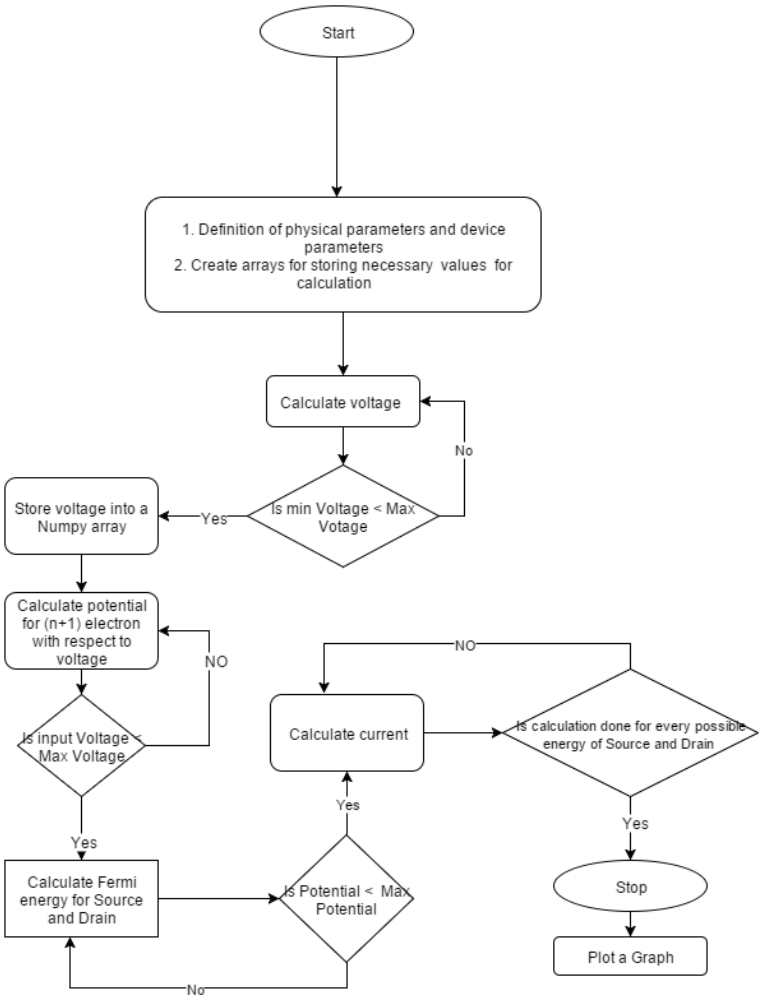

Figure 5.1: Flow diagram of python program used to calculate current

5.4 Sample Code

```
import matplotlib.pyplot as plt
import math
import numpy as np
import scipy.constants as con
from numpy import exp

#This array stores electrochemical potential
ecm=[]
ecm1=[]
ecm2=[]

############

#This array sotres Fermi energy for Drain Electrode
valuefd_1=[]
valuefd_2=[]
valuefd_3=[]      # Main Programme has more arrays. Here the item size
.............     # is reduced for space consumption,
                  # but the basic idea is same.
.............

############

#This array sotres Fermi energy for Source Electrode
value1=[]
valuefs_1=[]
valuefs_2=[]
valuefs_3=[]

.............     # Main Programme has more arrays. Here the item size
.............     # is reduced for space consumption,
                                # but the basic idea is same.
#######
```

```
# This array sotres Calculated current for individual scenario
current=[]
...........
............
# Main Programme has more arrays. Here the item size
# is reduced for space consumption, but the basic idea is same.

#########

# This stores the input voltage
voltage =[]

# Initial charging Voltage
charging_voltage=0


# Gate voltage connected to the island
gate_voltage1=2
gate_voltage2=2
gate_voltage3=2


# Pre-assigned Capacitance for Source, Drain, and Gate.
gate_capacitance =5*10**-18
source_capacitance=57*10**-18
drain_capacitance=38*10**-18

# Sum of three Capacitance
total_capacitance = gate_capacitance + source_capacitance + drain_capac

# Inputs Boltzmann Constant from scipy.constants
boltzman_constant =con.physical_constants["Boltzmann constant"]

#Inputs Charge of an Electron from scipy.constants
charge_of_an_electron = con.e

# Assigns Temperature in Kelvin
temperature =1
```

```
...........
............
# Main Programme has more arrays. Here the item size
# is reduced for space consumption, but the basic idea is same.
###############

# Calculates $k_{b}t$
thermal_energy =temperature*boltzman_constant[0]

...........
............
# Main Programme has more arrays. Here the item size
# is reduced for space consumption, but the basic idea is same.
###############


# This works as virtual Voltmeter. It gives values for certain interval
def _voltage_ (low,high,step):

    while low <=high:
        yield low
        low = low + step

for x in _voltage_((-1),(1),0.00001):
        voltage.append(x)


#############


# This function calculates the potential

def _ecmOfqdots_(voltage):
    for y in range(0,len(voltage)):

        ecm.append(float((-((((gate_voltage1-charging_voltage)
        *(gate_capacitance))+((source_capacitance)*(voltage[y])))
        /total_capacitance)*(charge_of_an_electron))))
```

```
# This methods calls the potential function and
# calculate the potential based on the input Voltage

_ecmOfqdots_(voltage)



#this loop calculates fermi state for source
# and store its value to a numpy list

for x in range (0,len(ecm)):
    value.append ((1+(np.exp((ecm[x]/thermal_energy))))**-1)



#this loop calculates fermi state for drain
# and store its value to a numpy list

for x in range (0,len(ecm)):
    value1.append ((1+(np.exp(((ecm[x]+
    (charge_of_an_electron*voltage[x]))/thermal_energy))))**-1)


#this loop calculates current

for i in range (0,len(ecm)):
    current.append((charge_of_an_electron * 10**9)
    *(value[i]-value1[i]))


print ("\*****Electrochemical potential for n+1 electron*********")
#print ecm
print ("\*******  Calculated Fermi value for source electrode *******")
#print value
print ("\*******  Calculated Fermi value for drain electrode *******")
#print value1
```

```
print ("\******* Current *******")
#print current

### Codes for Tuning, Shaping, Levelling The main Graph


plt.hold(True)
plt.plot(voltage,current, 'b-')
dpi = 800.0
xpixels, ypixels = 1200, 1200
plt.xlabel('Voltage (v)')
plt.ylabel('Current (I)')
plt.text(-0.2,10**-10, r'$T=0 \to 10 k$')
plt.text(-0.2,0.8*10**-10, r'$V = -5m\upsilon \to 5m\upsilon $')
plt.grid(True, lw = 0.7, ls = '-', c = '.75')
plt.show()
```

Chapter 6

Results

The ground state of Fermi-Dirac equation corresponds to absolute zero temperature. This section has a look at what happens to the system when the temperature becomes greater than zero. For non-zero temperature, the average number of fermions per single-particle state can be found from the so-called:

$$f_{FD} = \frac{1}{1 + \frac{E - E_f}{k_b T}}$$

This distribution is derived in chapter 1.3 and again in chapter 5.1 from different approach. Like the Bose-Einstein distribution for bosons, it depends on the energy E of the single-particle state, the absolute temperature T, the Boltzmann constant $k_b = 1.38 \times 10^{23} J/K$, and a chemical potential μ. In fact, the mathematical difference between the two distributions is merely that the Fermi-Dirac distribution has a plus sign in the denominator where the Bose-Einstein one has a minus sign. Still, that small change makes for very different statistics. The biggest difference is that f_{FD} is always less than one: the Fermi-Dirac distribution can never have more than one fermion in a given single-particle state. That follows from the fact that the exponential in the denominator of the distribution is always greater than zero, making the denominator greater than one.

It reflects the exclusion principle: there cannot be more than one

fermion in a given state, so the average per state cannot exceed one either. The Bose-Einstein distribution can have many bosons in a single state, especially in the presence of Bose-Einstein condensation.

Note incidentally that both the Fermi-Dirac and Bose-Einstein distributions count the different spin versions of a given spatial state as separate states. In particular for electrons, the spin-up and spin-down versions of a spatial state count as two separate states. Each can hold one electron.

Consider now the system ground state, that is predicted by the Fermi-Dirac distribution. In the limit that the temperature becomes zero, single-particle states end up with either exactly one electron or exactly zero electrons. The states that end up with one electron are the ones with energies E below the chemical potential μ. Similarly the states that end up empty are the ones with E above μ.

To see why, note that for $E - E_f < 0$, in the limit T the argument of the exponential in the Fermi-Dirac distribution becomes minus infinity. That makes the exponential zero, and f_{FD} is then equal to one. Conversely, for $E - E_f > 0$, in the limit T the argument of the exponential in the Fermi-Dirac distribution becomes positive infinity. That makes the exponential infinite, and f_{FD} is then zero.

The correct ground state, has one electron per state below the Fermi energy E_f and zero electrons per state above the Fermi energy. The Fermi-Dirac ground state can only agree with this if the chemical potential at absolute zero temperature is the same as the Fermi energy.

Next consider what happens if the absolute temperature is not zero but a bit larger than that. The story given above for zero temperature does not change significantly unless the value of $E - E_f$ is comparable to $k_b T$. Only in a energy range of order $k_b T$ around the Fermi energy does the average number of particles in a state change from its value at absolute zero temperature.

In physical terms, some electrons just below the Fermi energy pick up some thermal energy, which gives them an energy just above the Fermi energy. The affected energy range, and also the typical energy that the electrons in this range pick up, is comparable to $k_b T$. To good approximation,

the electrons always remain like they were in their ground state at $0K$.

One of the mysteries of physics before quantum mechanics was why the valence electrons in metals do not contribute to the heat capacity. At room temperature, the atoms in typical metals were known to have picked up an amount of thermal energy comparable to k_bT per atom. Classical physics predicted that the valence electrons, which could obviously move independently of the atoms, should pick up a similar amount of energy per electron. That should increase the heat capacity of metals. However, no such increase was observed.

The Fermi-Dirac distribution explains why only the electrons within a distance comparable to k_bT of the Fermi energy pick up the additional k_bT of thermal energy. This is only a very small fraction of the total number of electrons, so the contribution to the heat capacity is usually negligible. While classically the electrons may seem to move freely, in quantum mechanics they are constrained by the exclusion principle. Electrons cannot move to higher energy states if there are already electrons in these states.

6.1 Generated Current-Voltage Graph

Our simulation program assumes that we are using nano particle as source, drain and gate for transistor geometry. The temperature T we are taking is very below room temperature as nearly as absolute zero. For the sake of our observation we are keeping all the variable fixed, except gate voltage. The conditions we applied are $T = 1mK, E_0 = 0\,(V_c = 0)\,, (C_D : C_S : C_G = 38 : 57 : 5)$. From Fermi-Dirac distribution we can tell if $T \to 0$, $e^{\frac{E-E_f}{k_bT}}$ terms approaches to ∞ if $E < E_f$ and approaches to zero if $E < E_f$.

For $T = 0$:

$$f(e) = \begin{cases} 0 & \text{if } E > E_f \\ 1, & \text{if } E < E_f \end{cases}$$

We are applying this distribution function for our source and drain. Our program at very low temperature ($T = 1mK$) delivers us the result how current flows at different gate($V_g = 1mV, 2mV, 3mV$) voltage and within certain range of bias voltage. We plot current vs voltage graph it shows the result as below.

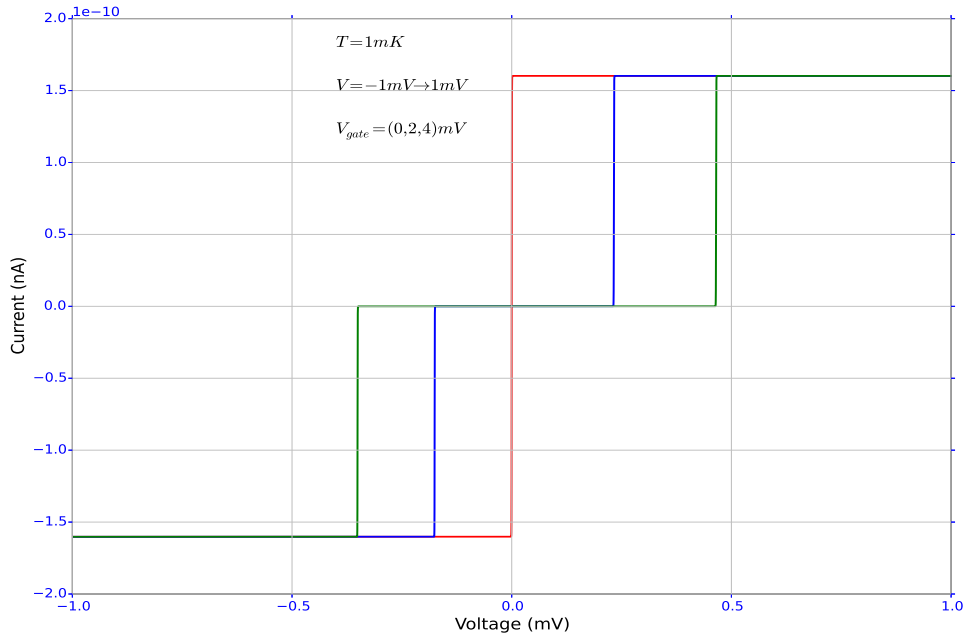

Figure 6.1: Three I-V taken at different $V_g s$. They show a conductance suppressed region near zero bias followed by a current step.

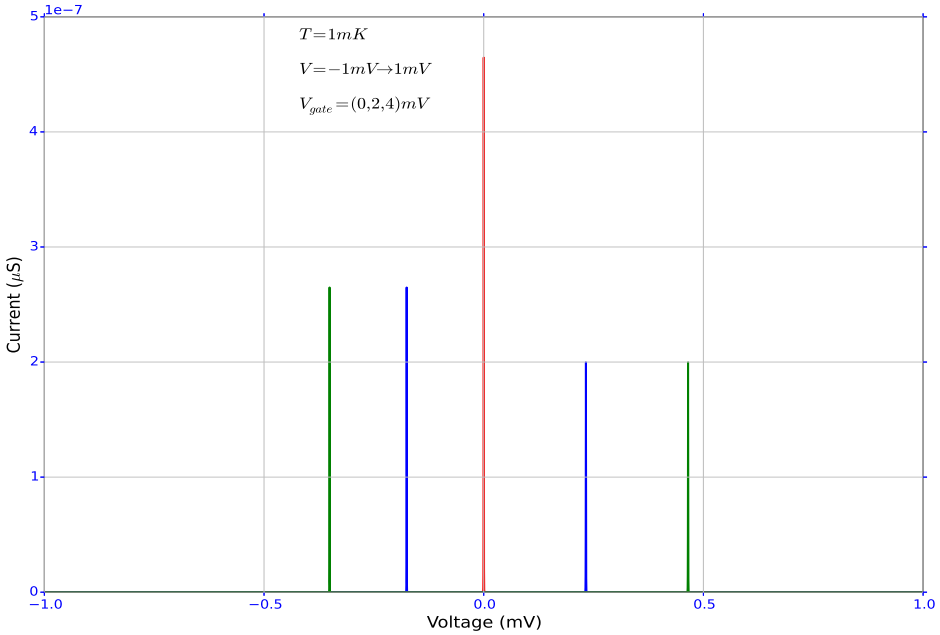

Figure 6.2: $\frac{dI}{dV}$ as a function of V. They show peaks corresponding to current steps in fig- 6.1

6.2 Maximum Size and Temperature

Since our simulation program can show the variance in current with respect to increasing voltage, we extend our program such a way so that we can add temperature as an variable. It shows us, as we assumed that the increasing temperature breaks the discreteness nature of current flow. We observed that at $2.5K$(approximately) the discreteness nature of current flow started to vanish and gradually it falls into classical regime. However at $7K$ the curve becomes so continuous it appeared as well-known Ohm's current-voltage curve and discreteness completely vanishes. From that speculation, using the Schrodinger equation for spherical dot and the condition for charge addition energy $\Delta E \gg k_b T$ we tried to calculate the maximum size of the quantum dot. Another very important point we should keep in mind is that we assumed very simplified model in order to calculate the radius of quantum dot such as our quantum dot is qhighly symmetrical cubic box and we only calculate the energy from ground level to the first excitation level. We ignore other excitation level but in our simulation we allow all possible level. Now let us assume that the box has edge-length L and occupies the the region $0 < x, y, z < L$. We assume the box walls are smooth. So particles exerts forces only perpendicular to the surface.

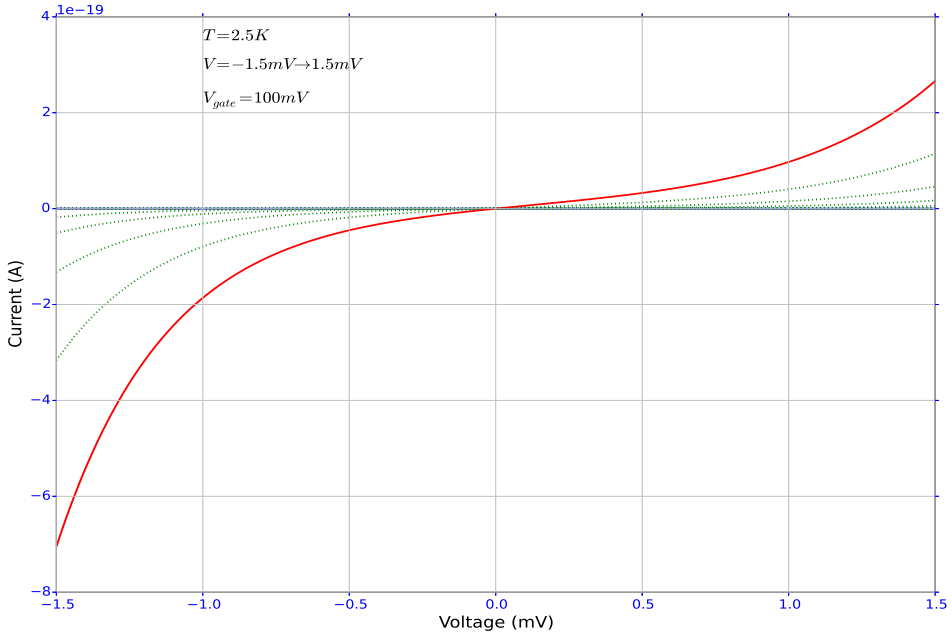

Figure 6.3: $IvsV$ graph at increasing temperature

Now for the sake of simplicity and to be remain in the safe side we took $2.5K$ as the breaking point at which the discreteness or Coulomb staircase completely disappear. So the energy of ground state would be as below :

$$\begin{aligned} E_{111} &= \frac{3\pi^2\hbar^2}{2mL^2} \\ &= \frac{3h^2}{8mL^2} \end{aligned}$$

Since first excitation level has three possible states we can write energy for first excitation level:

$$E_{112} = E_{121} = E_{211} = \frac{6\pi^2\hbar^2}{2mL^2}$$
$$= \frac{6h^2}{8mL^2}$$

Now ΔE would be the difference of two state which is :

$$\Delta E = \frac{6h^2}{8mL^2} - \frac{3h^2}{8mL^2}$$
$$= \frac{3h^2}{8mL^2}$$
$$= \frac{3 \times (6.2607 \times 10^{-34})^2}{8 \times (9.11 \times 10^{-31}) \times L^2}$$

Again using the charging condition we can write $\Delta E > k_b T$. Therefore :

$$k_b t < \frac{3 \times (6.2607 \times 10^{-34})^2}{8 \times (9.11 \times 10^{-31}) \times L^2}$$
$$L < \sqrt{\frac{3 \times (6.2607 \times 10^{-34})^2}{8 \times (9.11 \times 10^{-31}) \times k_b T}}$$
$$< \sqrt{\frac{3 \times (6.2607 \times 10^{-34})^2}{8 \times (9.11 \times 10^{-31}) \times (1.380 \times 10^{-23}) \times 2.5}}$$
$$< 68.38640 \times 10^{-9} m$$

So this L is the maximum edge-length of our simplified and highly symmetric cubic quantum dot.

Chapter 7

Conclusions and Further Research

Now a days smiluating a physics problem or experimenting a well defined physical theory using a computer is easier and less costly than doing it in a Laboratory. Accuracy in computer measurement could be better than the real experiment if we could design model of the problem by taking in consideration all the variables that take part in real life experiment. Finding all the variable that governs the model of the problem including those imposed by environment itself and understanding them how it connect all the conceptual dots in order to visualize them into a computer program has been remained as incomplete in my thesis. On the other hand computational speed of my computer against large data handling was quite into downward direction .Therefore I have to, sadly neglect all the minor variables and consider a very ideal scenario while modelling the system. It would be more accurate while calculating current for a bulk material if we could virtually construct a real bulk metal consisting every atom. We might be able to build an atom with all the electron inside it and then bind those atom according to their atomic structure.This virtual metal would not contain any defects like real metal but it could act like a real metal and hopefully provide us very good result. So at first we badly wanted to design such model but in reality we saw that using a normal home desktop pc it was quite impossible. It could not be possible for me since the unavailability of such platform. Therefore our

future plan is to build a cluster computer with multiple processor and then develop a complete solution for nano particles so that we could construct a nearly complete model of electronic transportation in nano particles at very low temperature using well tuned parameter. In our simulation due to computational speed and lack of prerequisite knowledge we sometimes ignored real data although we did not want to. In the next step our main concern would be not to arise these kind of scenarios and also wish to minimize the lack of prerequisite knowledge.

List of Figures

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